Atomic and Molecular Physics for Astronomical Observations

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Layout of Talk

- Overview of SciDAC (Scientific Discovery through Advanced Computing) project to provide atomic data for use by fusion plasma modelers
  - Atomic data provision and formats
  - Electron-impact excitation
  - Electron-impact ionization
  - Dielectronic recombination
  - Other atomic physics calculations (spin-offs!)
- Recent/current atomic scattering calculations relevant to astrophysics
- Some planned projects of relevance
- Discussion of the current atomic data needs of astrophysics

Terascale computational atomic physics for controlled fusion energy

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Atomic Data Provision

- *Controlled Fusion Atomic Data Center at Oak Ridge National Laboratory, TN*
- *http://www-cfadc.phy.ornl.gov*

- ***A**tomic **D**ata and **A**nalysis **S**tructure, UK consortium based at Strathclyde University, Glasgow, UK, and JET, Oxford, UK*
- *http://adas.phys.strath.ac.uk/adas/docs/manual*
- **H. P. Summers, ADAS Users Manual (2nd Edition) (2003)**

Scientific Utilization of Advanced Computing Platforms

- **Address fundamental problems in atomic and molecular physics**
  - *One-center three-body break-up problem*
  - *Two-center two-body scattering problems*
  - *Collisions in intense external fields*

- **Respond to current needs in controlled fusion energy**
  - *Lithium database for DIII-D plasma transport codes*
  - *Beryllium database for wall component studies at UCSD (PISCES)*
  - *Heavy species database for wall erosion studies at JET*

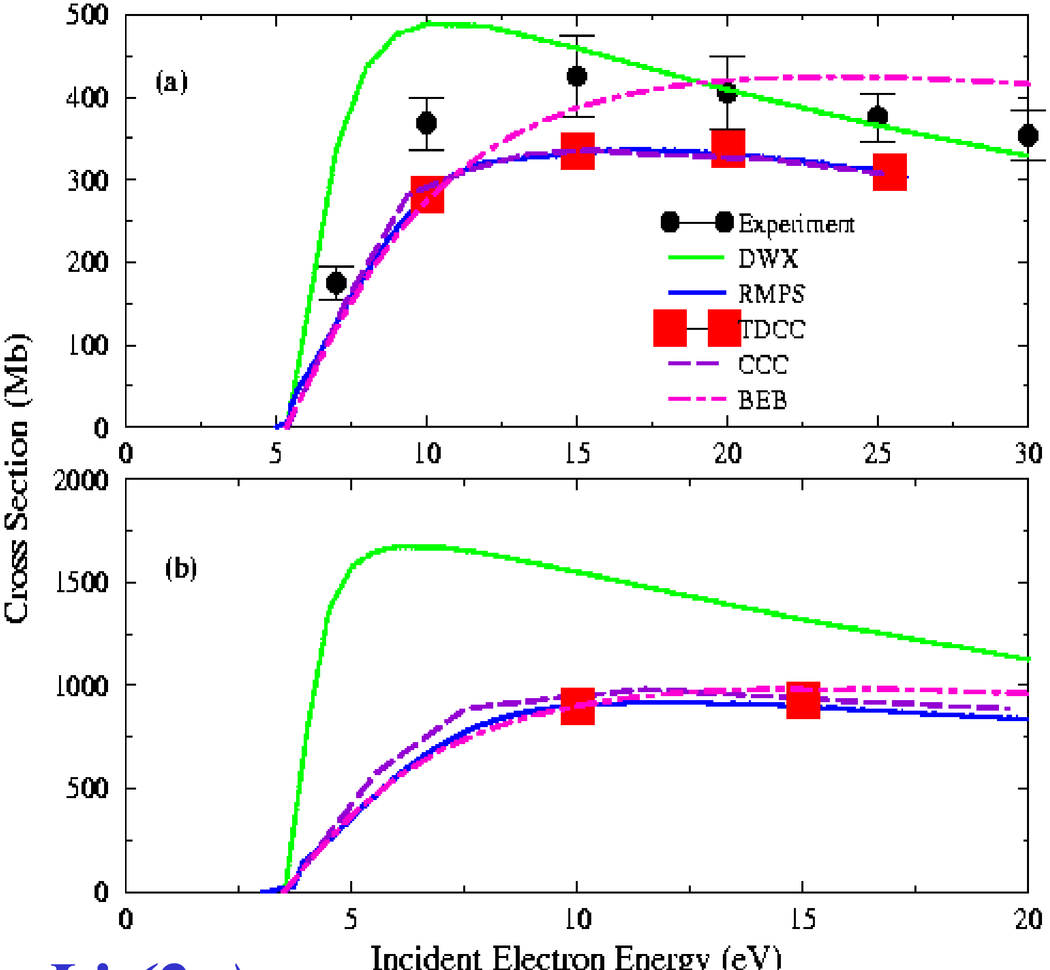
- **Apply computational methods to other scientific areas**
  - *Simulations of cold Rydberg plasmas*
  - *Time-dependent studies of Bose-Einstein condensates*
  - *Iron spectral analysis of active galactic nuclei*

Electron-Impact Ionization Data for modeling fusion plasmas

- Program initiated several years ago to completely revise electron-impact excitation and ionization data for lithium
- Excitation and ionization of Li, Li^+, Li^{2+} examined
- Significant differences found between our TDCC calculations and experiment for neutral Li
- Three non-perturbative techniques however gave excellent agreement for Li – suggest experimental measurements need revision
- Data placed in format suitable for use by astrophysical (and fusion) plasma modelers
- Will be used to support plasma edge diagnostics made using a Li beam at the DIIID tokamak in San Diego (GA)

Electron-impact ionization of lithium

Li (2s)



Li (2p)

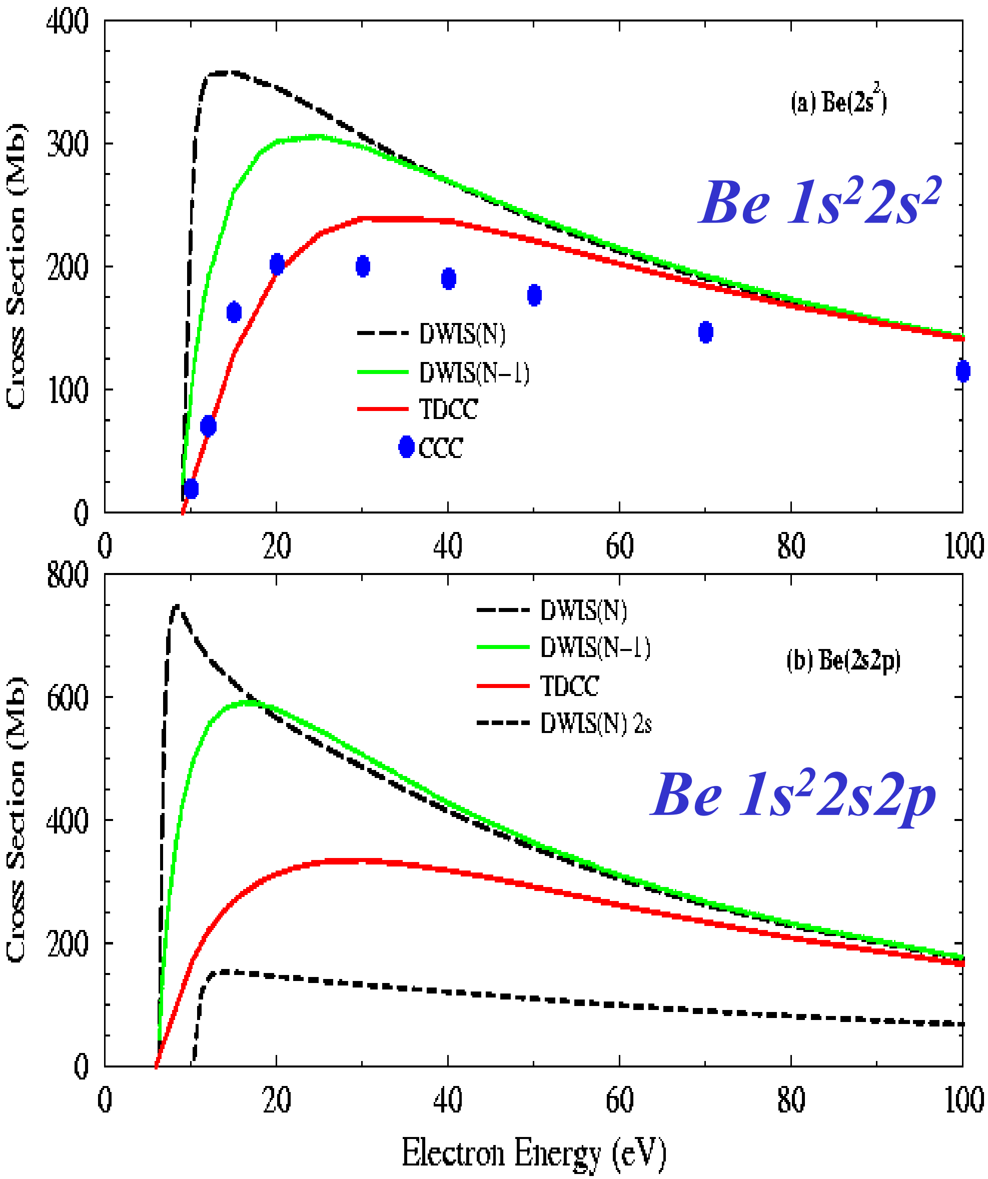
Demonstrates importance of treating three-body Coulomb problem using non-perturbative methods – large differences with perturbative calculations of 50 – 100 % in ionization cross section

J. Colgan, M. S. Pindzola, D. M. Mitnik, D. C. Griffin, and I. Bray, Phys. Rev. Letts. 87, 213201 (2001)

Electron-Impact Ionization Data for modeling plasmas

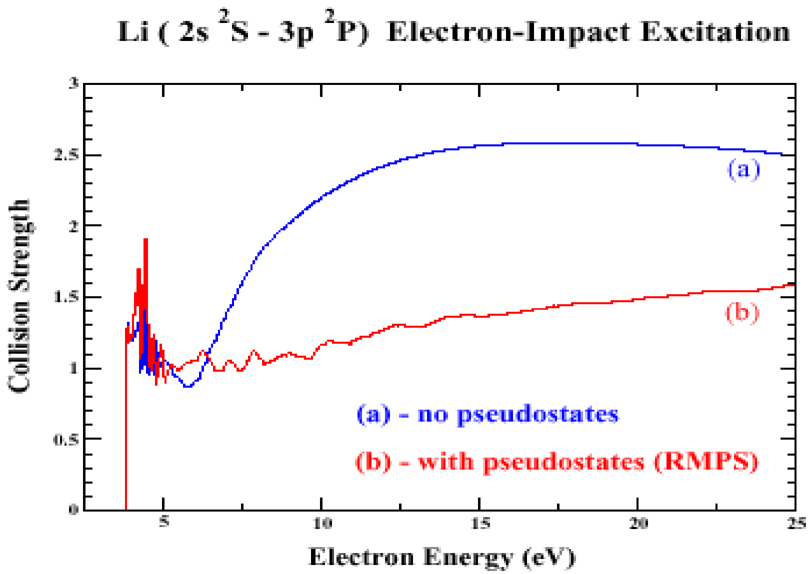
- Program currently underway to revise electron-impact excitation and ionization data for beryllium
- Recently calculated electron-impact ionization of Be, Be^{+}, Be^{2+}, and Be^{3+}. Excitation calculations well underway
- Few experimental measurements due to toxicity of beryllium
- Significant differences found between TDCC calculations and perturbative distorted-wave calculations for neutral Be
- Differences between non-perturbative and perturbative decrease as ion stage increases
- Data placed in format suitable for use by astrophysical (and fusion) plasma modelers – specifically for the PISCES plasma fusion device at UCSD which will use Be as a potential plasma-facing wall component

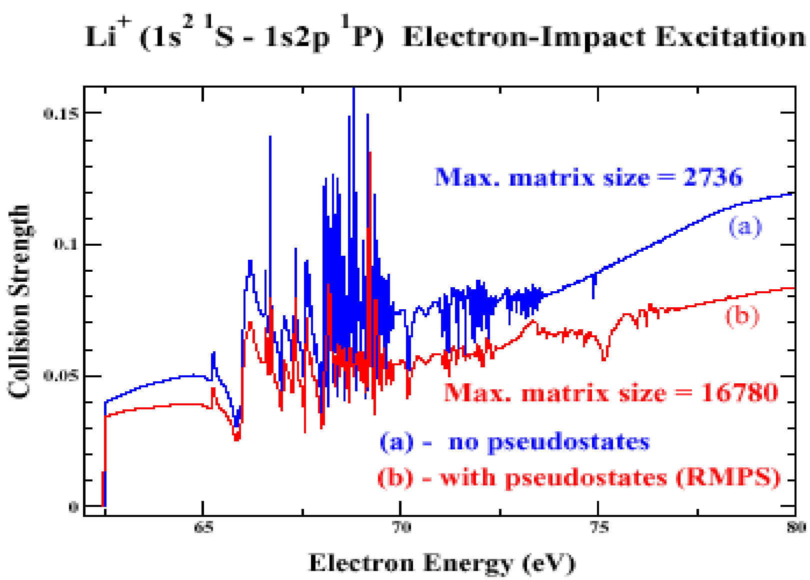
Electron-impact ionization of Be



- **Red line: TDCC**
- **Green line: DWIS(N)**
- **Black line: DWIS(N-1)**
- **Blue circles: CCC**
- Large differences near ionization threshold and cross section peak between the perturbative and nonperturbative calculations
- No experimental measurements with which to compare for either configuration
- ***J. Colgan, S. D. Loch, M. S. Pindzola, C. P. Ballance, and D. C. Griffin, Phys. Rev. A, submitted (2003).***

Electron-impact excitation of Li and Li^+



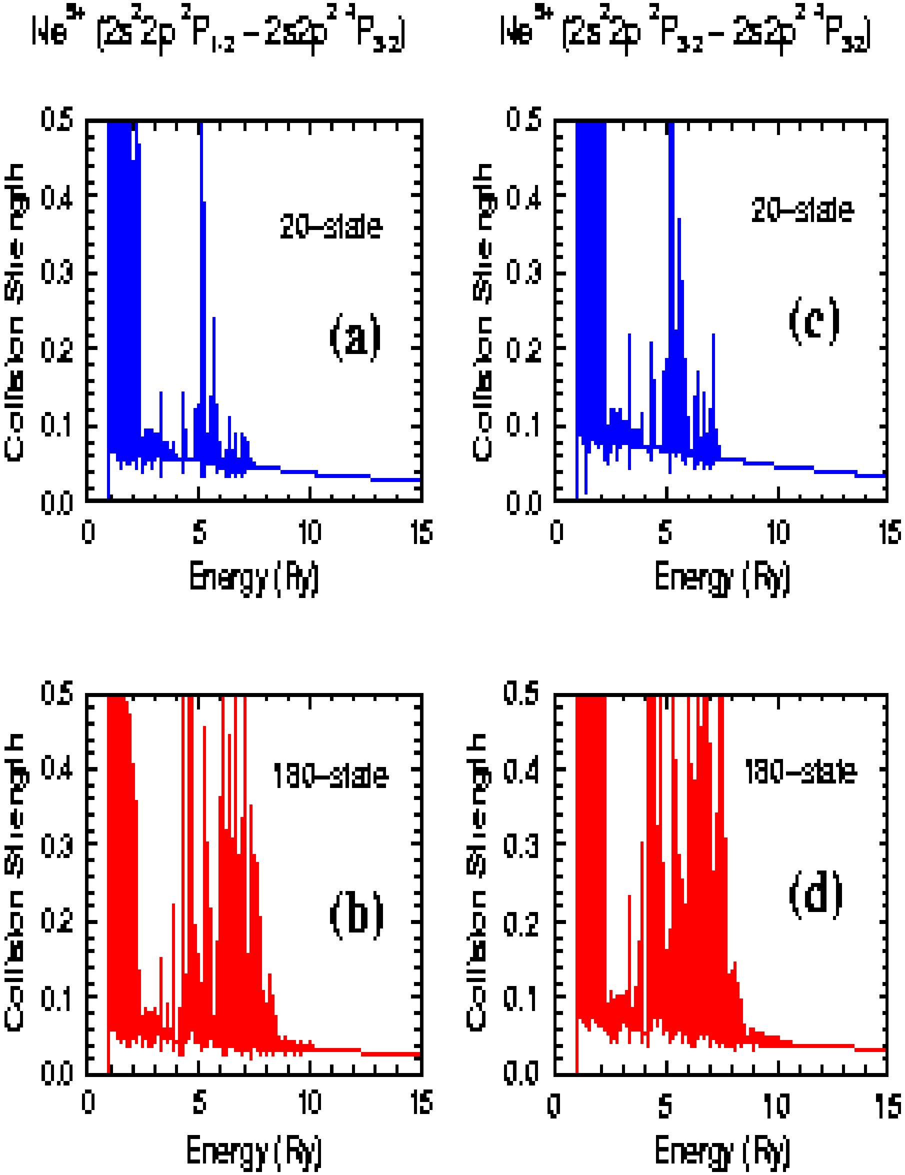


- R-matrix with Pseudo States (RMPS) method has been used for many electron-impact excitation cross section calculations:

- In these calculations use of pseudo states reflected the importance of accurately representing the coupling to the continuum

- **Li**: D. C. Griffin et al, Phys. Rev. A **64**, 032718 (2001).
- **Li^+**: C. P. Ballance et al, J. Phys. B **36**, 235 (2003).
- **C^{2+}**: D. M. Mitnik et al, J. Phys. B **36**, 717 (2003).
- **C^{3+}**: D. C. Griffin et al, J. Phys. B **33**, 1013 (2000).

Electron-impact excitation of heavier ions



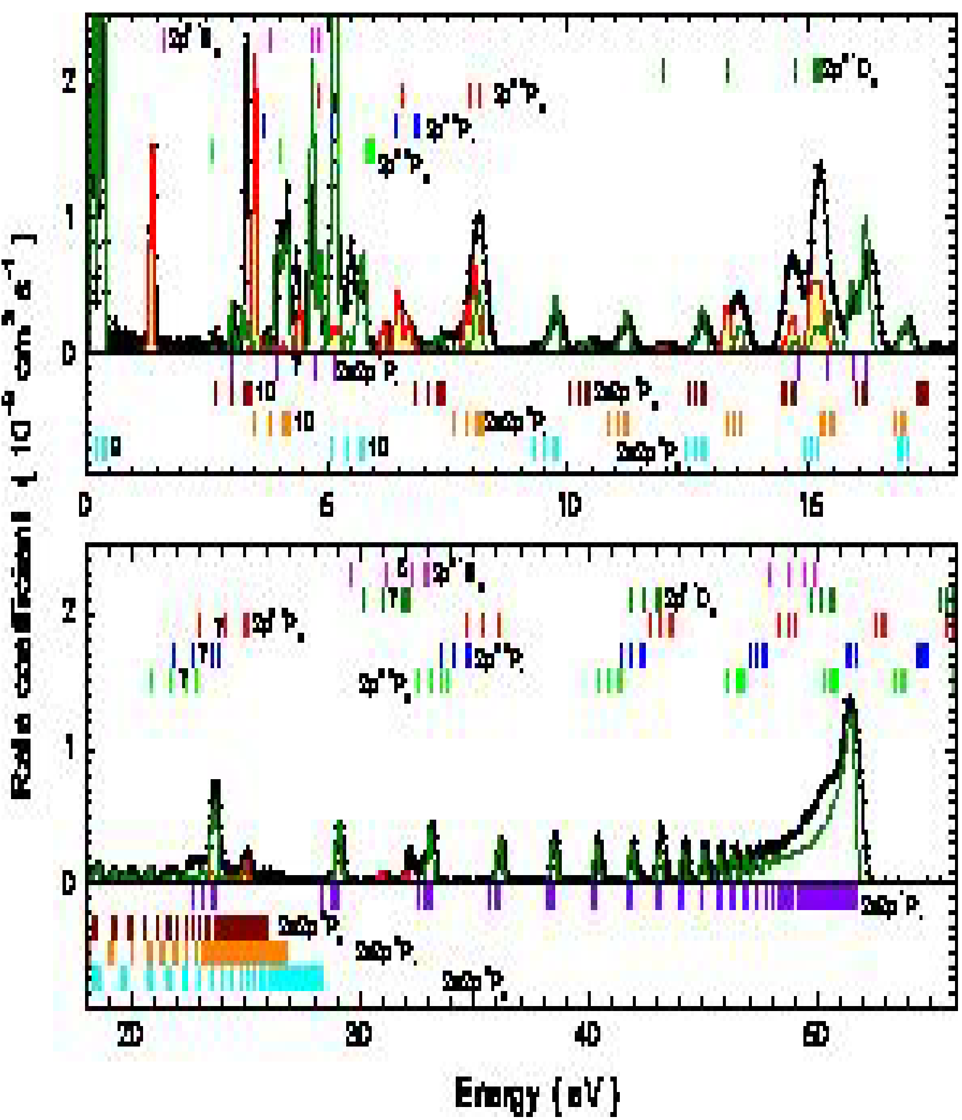
- Large R-matrix calculations (with no pseudo states) contain many levels to represent the low-lying bound states accurately
- Ne^{+}: Griffin et al, J. Phys. B **34**, 4401 (2001).
- Ne^{4+}: Griffin et al, J. Phys. B **33**, 4389 (2000).
- Ne^{5+}: Mitnik et al, J. Phys. B **34**, 4455 (2001).
- Fe^{20+}: Badnell and Griffin, J. Phys. B **34**, 681 (2001).
- Fe^{21+}: Badnell et al, J. Phys. B **34**, 5071 (2001).
- Fe^{23+}: Whiteford et al, J. Phys. B **35**, 3729 (2002).
- Fe^{24+}: Whiteford et al, J. Phys. B **34**, 3179 (2002).
- Fe^{25+}: Ballance et al, J. Phys. B **35**, 1095 (2002).

Dielectronic Recombination

- Project well underway to calculate dielectronic recombination rate coefficients for complete isoelectronic sequences
- Currently completed H-like through Ne-like sequence;
- Moving onto second row of periodic table
- Theoretical approach is more accurate at high temperatures where recombination is more focused towards fusion plasma applications

- ***Theory & Methodology: N. R. Badnell et al, A&A, accepted (2003).***
- ***H-like: N. R. Badnell et al, A&A, submitted, (2003).***
- ***He-like: N. R. Badnell et al, A&A submitted, (2003).***
- ***Li-like: J. Colgan, M. S. Pindzola, and N. R. Badnell, A&A, submitted (2003).***
- ***Be-like: J. Colgan, M. S. Pindzola, A. D. Whiteford, and N. R. Badnell, A&A, submitted (2003).***

Dielectronic Recombination of Cl^{13+}

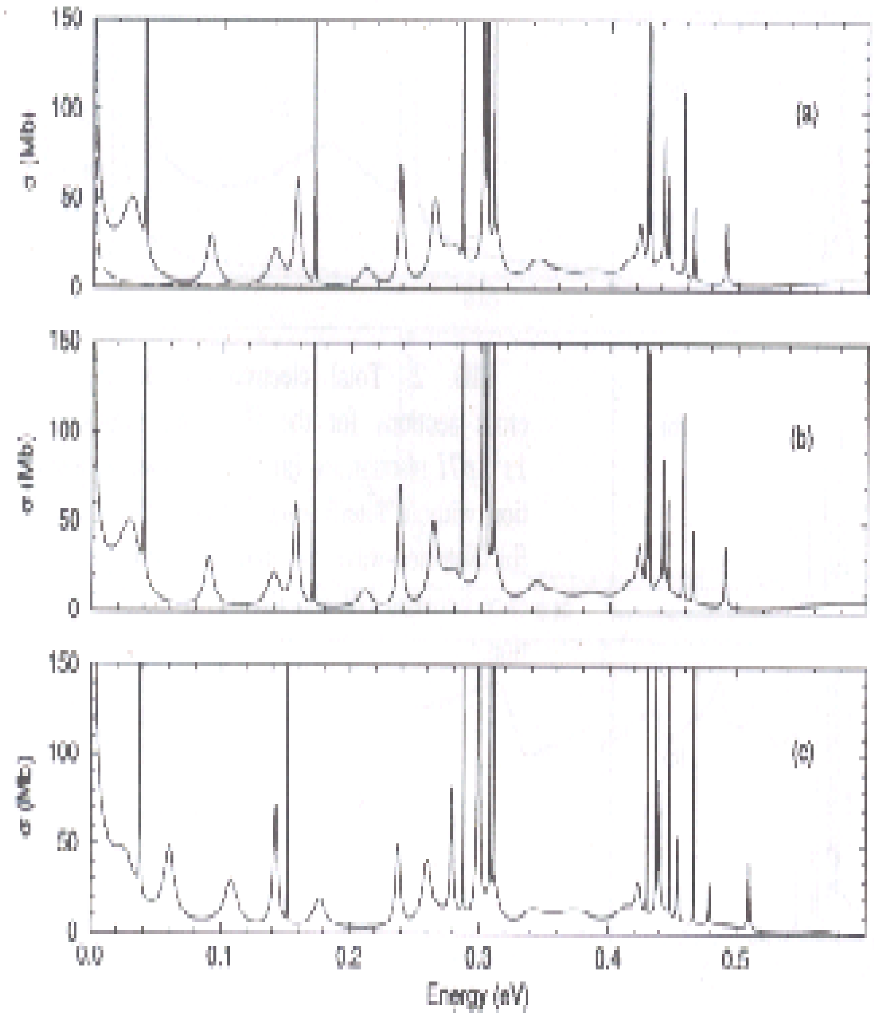


- Dielectronic recombination rate coefficients for Be-like Cl^{13+}
- Comparisons of our theoretical calculations with experiment of Heidelberg group at the TSR
- Experimental confirmation of DR project results
- Trielectronic recombination (core excitation of two electrons) observed for the first time

- ***M. Schnell et al. Phys. Rev. Lett. 88, XXXXXX (2003).***

Problems for low temperature Dielectronic Recombination

F^{6+}



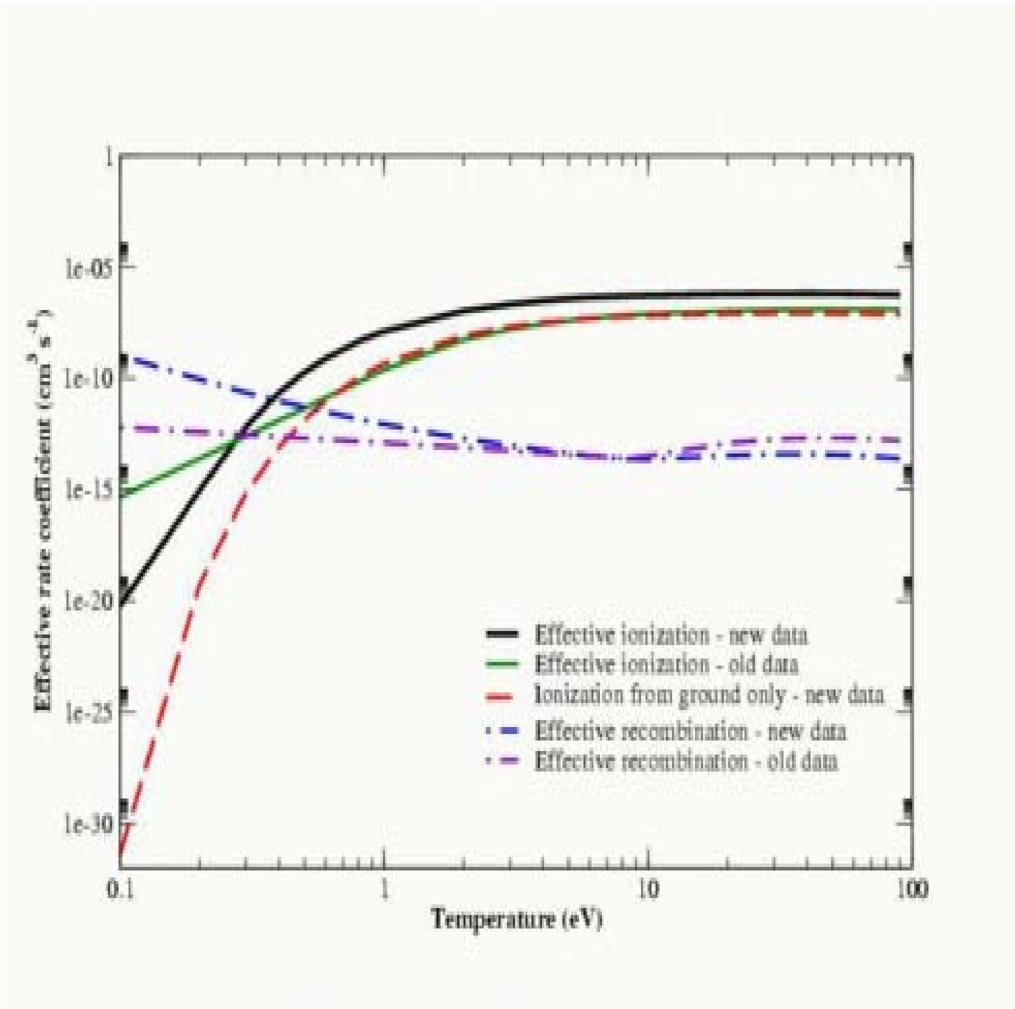
- a) DW calculations with no interference
- b) DW calculations with interference
- c) *R*-matrix calculation

- Very large structure calculations necessary to get position of resonances correctly
- Also need to include effects of interference between radiative and dielectronic recombination
- Also the effect of interacting resonances on recombination
- ***Expt/theory for C^{3+}: S. Mannervik et al, Phys. Rev. Lett. 81, 313 (1998).***
- ***Theory for F^{6+}: D. M. Mitnik, M. S. Pindzola, and N. R. Badnell, Phys. Rev. A 59, 3592 (1999).***
- ***Expt/theory for F^{6+}: M. Tokman et al, Phys. Rev. A 66, 012703 (2002).***

Problems for high temperature Dielectronic Recombination

- Near Rydberg limits weakly bound states can be strongly affected by electric and/or magnetic fields present. The plasma microfield and the plasma densities near threshold can also have a strong influence on the rates in these regions
- Calculations which take into account interacting resonances and DR in crossed electric and magnetic fields have been made:
  - ***model calculation: F. Robicheaux and M. S. Pindzola, Phys. Rev. Lett. 79, 2237 (1997).***
  - ***C^{3+}, Si^{11+}: F. Robicheaux, M. S. Pindzola, and D. C. Griffin, Phys. Rev. Lett. 80, 1402 (1998).***
  - ***C^{6+}, F^{6+} expt: G. Gwinner et al, Phys. Rev. Lett. 84, 4822 (2000).***
  - ***O^{5+} expt/theory: S. Bohm et al, Phys. Rev. A 65, 052728 (2002).***
- Currently no generalized codes exist which take into account crossed field effects within a detailed structure calculation
- These huge calculations will require parallelization of existing recombination computer codes

Effective ionization rates for Li

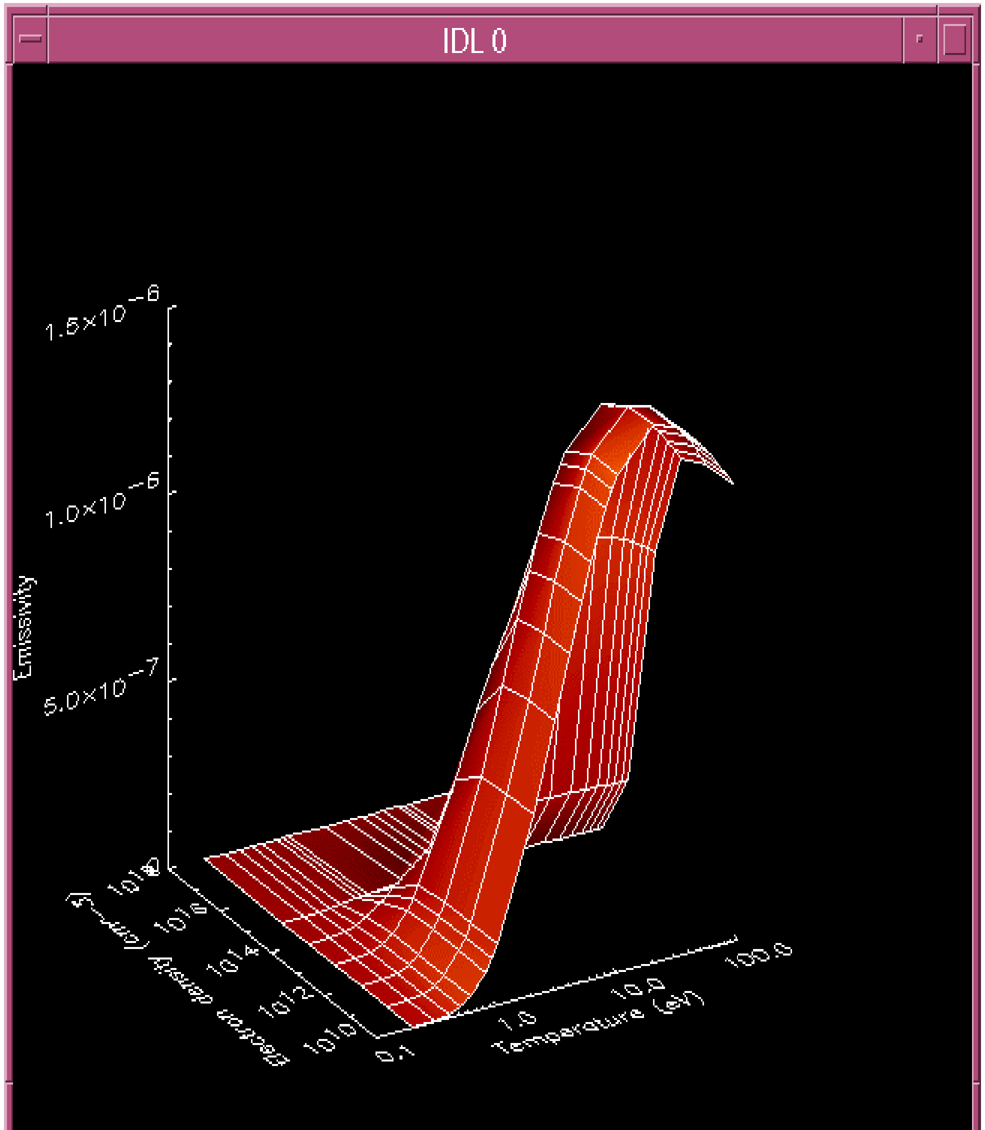


Effective ionization rate for Li at an electron density of 10^{14} cm^{-3} as a function of electron temperature

- New data for excitation, ionization, and recombination has been incorporated into an ADAS plasma modeling calculation
- Also available at CFADC database
- Very large differences compared to model using older atomic data
- Significant increase in the accuracy of the plasma modeling for lithium

- ***S. D. Loch et al, Physica Scripta, submitted (2003).***

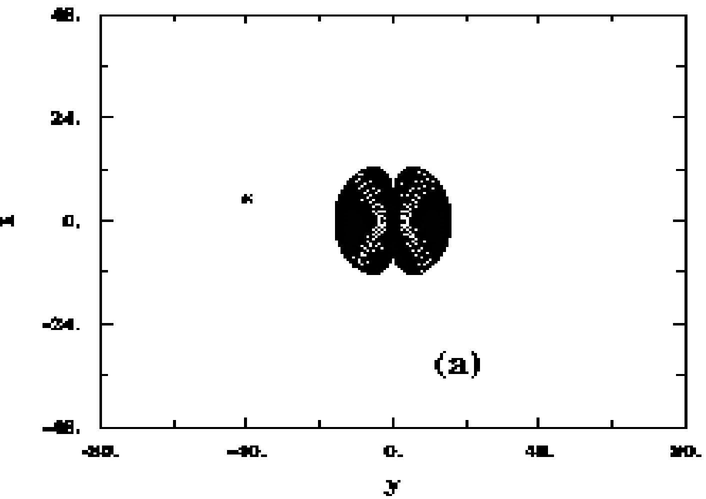
Li emissivity coefficients

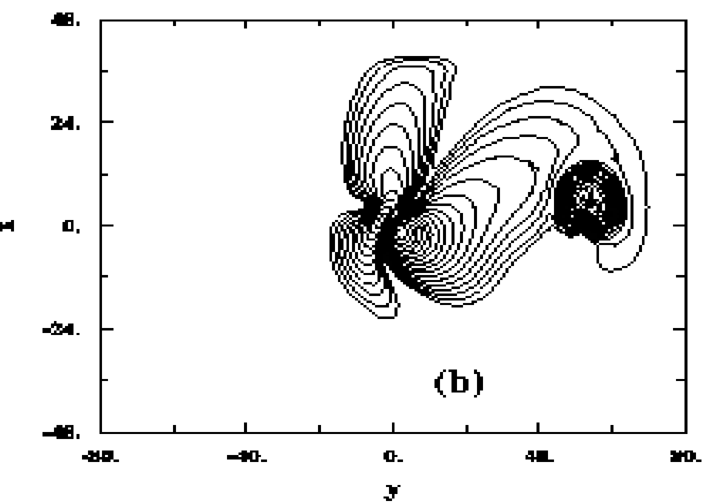


- Emissivity coefficients as a function of electron temperature and density
- Obtained from ADAS modeling calculation
- Data such as this is used in a wide range of fusion plasma edge diagnostics
- Also comparing these and similar plasma characteristics with modeling calculations made using Los Alamos set of computer codes

- ***S. D. Loch, C. Fontes et al, Phys. Rev. E, submitted, (2003).***

Ion-Atom Collisions

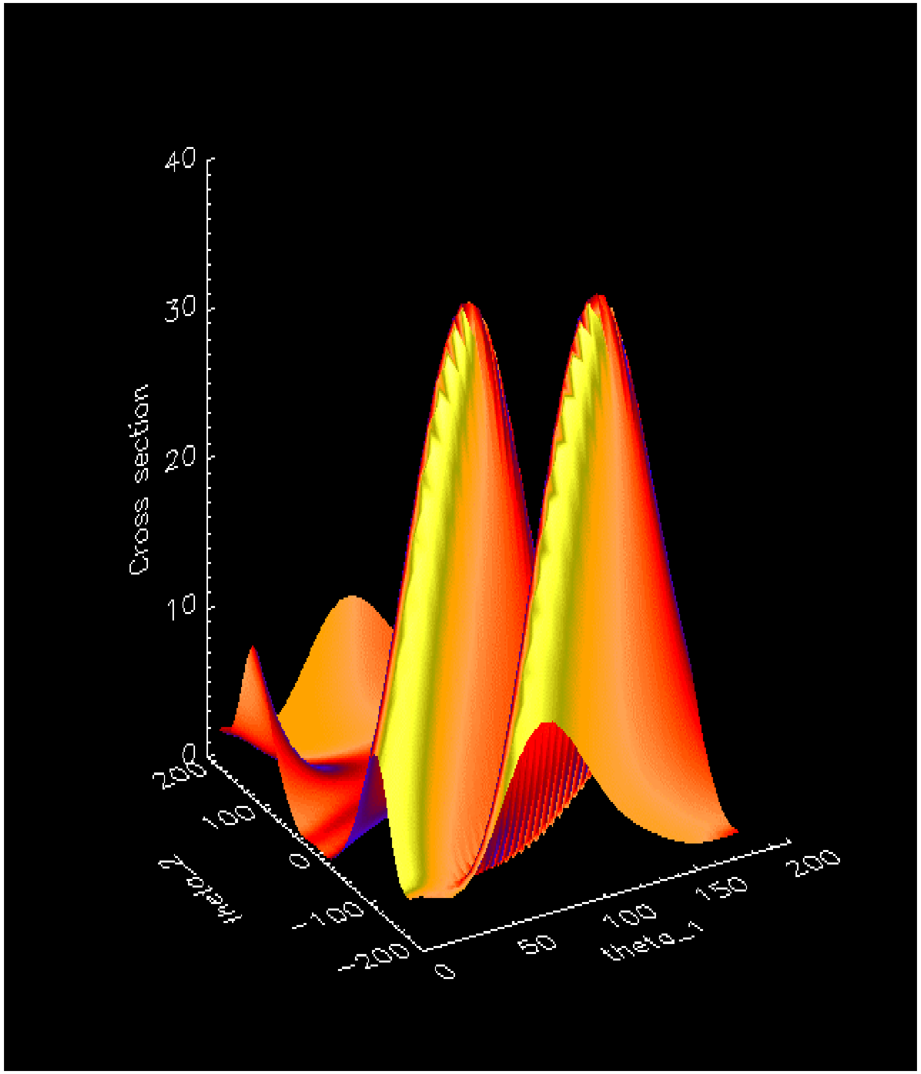




Time-dependent evolution of electronic wave function during collision

- *p + H:* D. R. Schultz, et al, Phys. Rev. Lett. **76**, 2882 (1996).
- *p + H:* J. C. Wells, et al, Phys. Rev. A **54**, 593 (1996).
- *p + H:* A.Kolakowska, et al, Phys. Rev. A **58**, 2872 (1998).
- *p + H:* D. R. Schultz, M. R. Strayer, and J. C. Wells, Phys. Rev. Lett. **82**, 3976 (1999).
- *p + Li:* M. S. Pindzola, Phys. Rev. A **60**, 3764 (1999).
- *p + Li*:* M. S. Pindzola, Phys. Rev. A **66**, 032716 (2002).
- *α + H:* M. S. Pindzola, T. Minami, and D. R. Schultz, Phys. Rev. A **68**, XXXXXX (2003).
- Currently working on:
  - *Be^{4+} + H:*
  - *p + H*: in ExB fields*

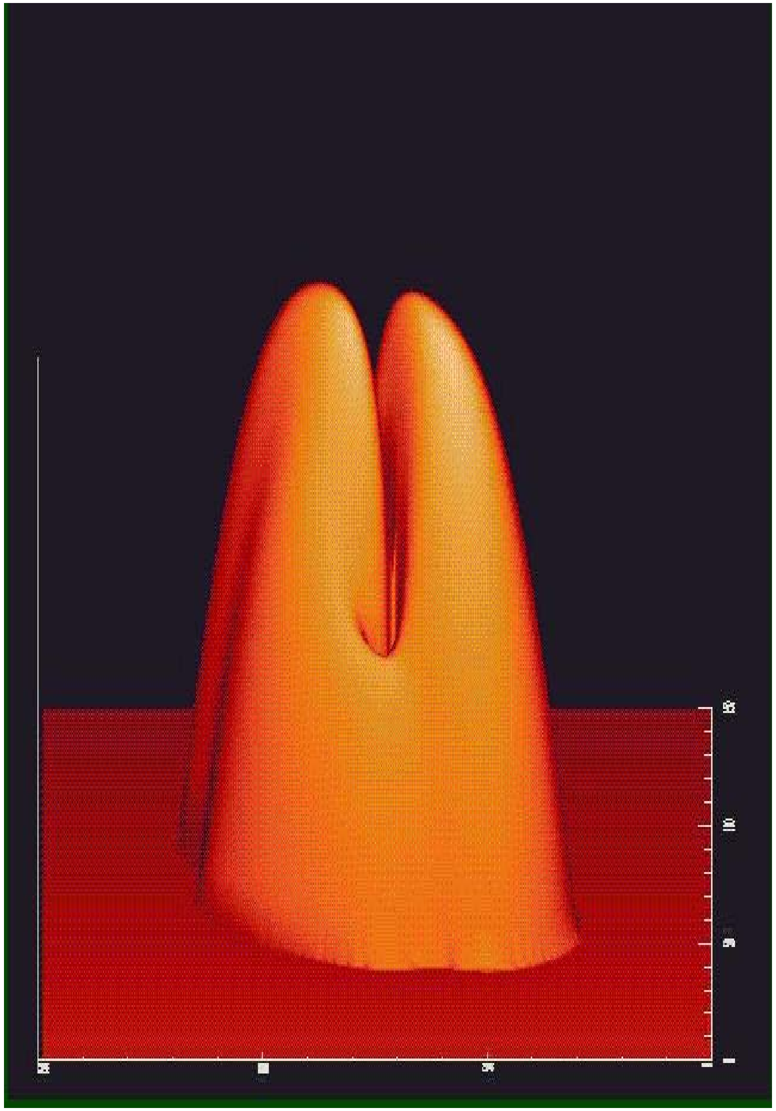
Double photoionization of helium



- *(γ,2e)* **He:** J. Colgan, M. S. Pindzola, and F. Robicheaux, J. Phys. B **34**, L457 (2001).
- *(γ,2e)* **He:** J. Colgan and M. S. Pindzola, Phys. Rev. A **65**,032729 (2002).
- *(γ,2e)* **Be:** J. Colgan and M. S. Pindzola, Phys. Rev. A **65**, 022709 (2002).
- *(2γ,2e)* **He:** J. Colgan and M. S. Pindzola, Phys. Rev. Lett. **88**, 173002 (2002)
- *(γ,2e)* **He*:** J. Colgan and M. S. Pindzola, Phys. Rev. A **67**, 012711 (2003).

Triple differential cross section at equal energy sharing between the ejected electrons

Mode excitation of a BEC soliton state



Density plot of a sodium condensate in a soliton state undergoing mode excitation

- D. L. Feder, M. S. Pindzola, L. A. Collins, B. I. Schneider, C. W. Clark, Phys. Rev. A **62**, 053606 (2000).
- J. Denschlag et al, Science **287**, 97 (2000).
- M. S. Pindzola and F. Texier, J. Phys. B **36**, XXX (2003).

- Currently working on BEC's in wave-guides in collaboration with the MIT group of Pritchard and Ketterle.

Simulations of ultra-cold plasmas

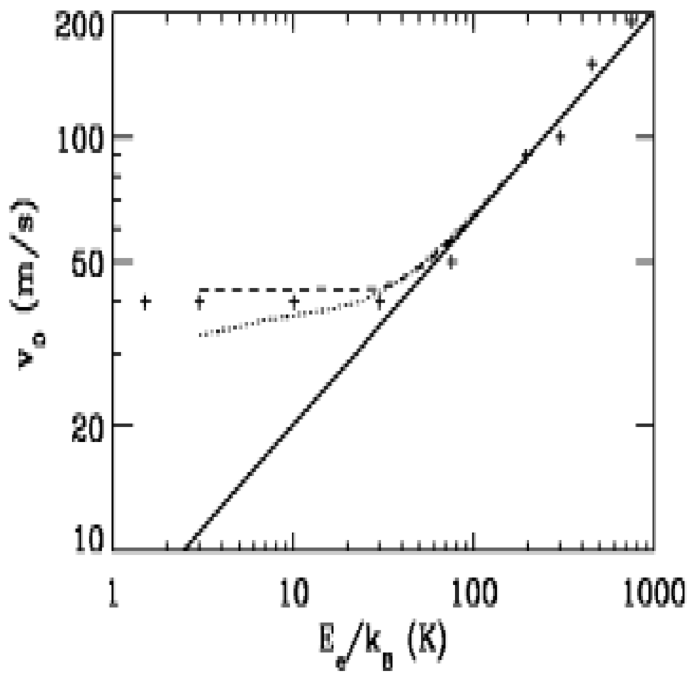


FIG. 2. Asymptotic expansion velocity, v_0, as defined in Ref. [2] as a function of the initial energy per ion. The crosses indicate representative experimental results [2]. The solid line is with no three-body recombination. The dotted line is with three-body recombination but no electron-Rydberg atom scattering. The dashed line is with three-body recombination and electron-Rydberg scattering. The calculations are for the initial average density of $n_e = 10^{15}$ m^{-3}.

•F. Robicheaux and J. D. Hanson, Phys. Rev. Lett. **88**, 055002 (2002).

•F. Robicheaux and J. D. Hanson, Phys. Plasmas **10**, June (2003).

Inclusion of electron-Rydberg scattering and three-body recombination is necessary to properly simulate the expansion of an ultra-cold plasma

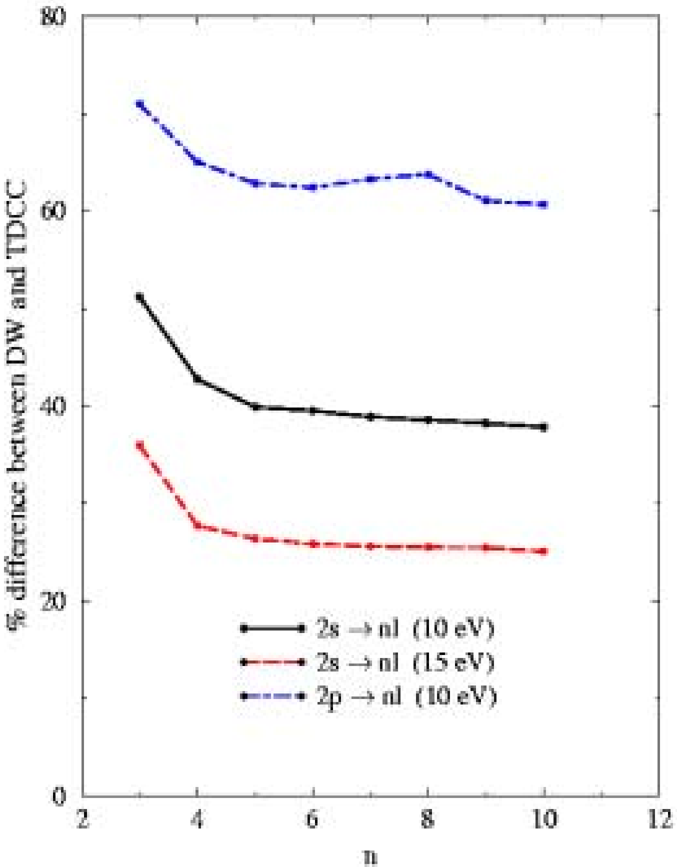
E.g.: Supernova remnants (SNR's)

- Recent successful modeling of nebular spectra in Type Ia supernovae by including forbidden lines of cobalt ions
- Electron-impact excitation cross sections calculated using distorted-wave and *R*-matrix calculations for transitions in Co^{2+}
- ***W. Liu, D. J. Jeffery, D. R. Schultz, P. Quinet, J. Shaw, and M. S. Pindzola, Ap. J 489, L141 (1997).***
- ***J. Shaw, M. S. Pindzola, N. R. Badnell, and D. C. Griffin, Phys. Rev. A 58, 2920 (1998).***

The Crab Nebula – one of the earliest recorded Supernova explosions

E.g.: Early Universe abundances of ^4He and ^7Li

Electron-impact excitation of neutral Li from 2s and 2p to high quantum number n

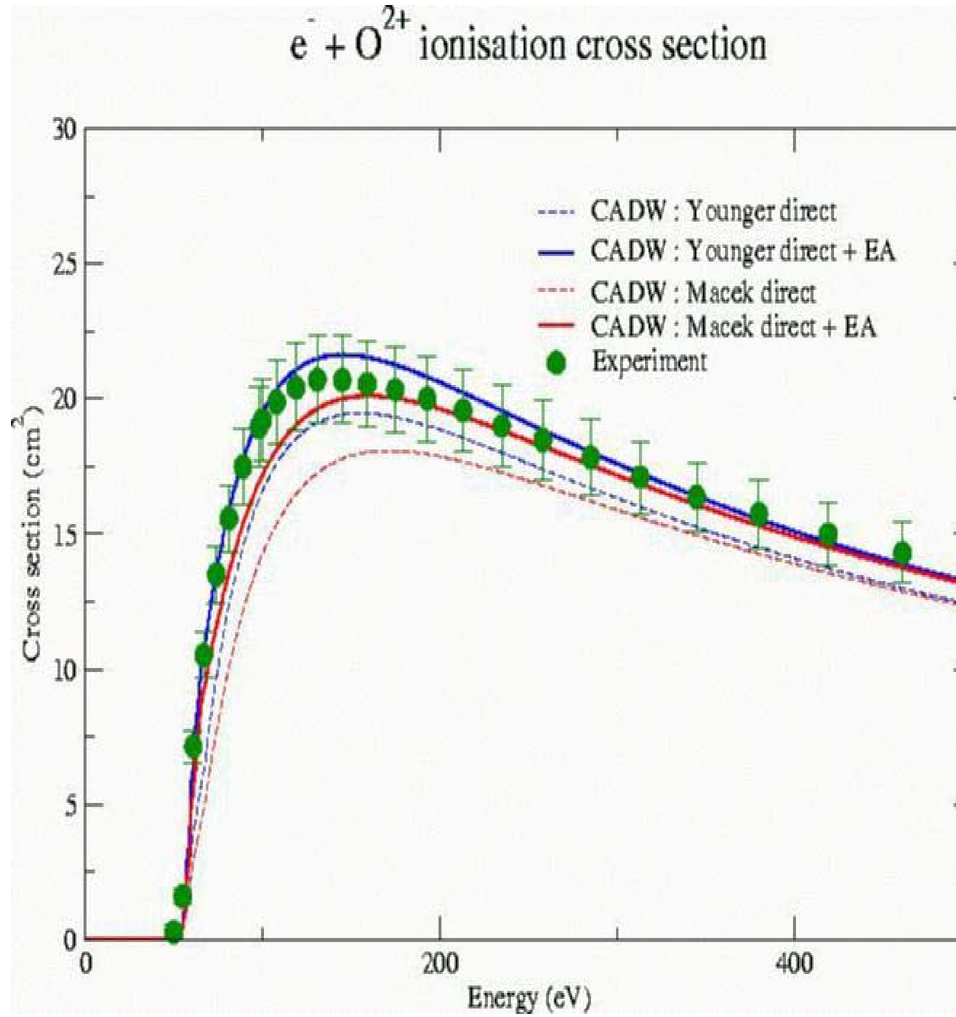


- At low energies, TDCC method is around 50% different from DW calculations for excitation to all n-manifolds for Li and He^+ systems
- Current databases use (at best) perturbative (DW) methods for these transitions – these may be in error by almost a factor of 2
- Working with G. Ferland to improve quality of He and Li atomic data used in astrophysical models

- ***He^+: M. C. Witthoeft, M. S. Pindzola, and J. Colgan, Phys. Rev. A 67, 032713 (2003).***
- ***Li: M. C. Witthoeft, J. Colgan, and M. S.***

E.g.: Cometary X-ray emissions

- X-rays have been observed from many comets and their origin is still unclear
- Some unified plasma models explain this by modified two stream instabilities – Kellet et al
- However, they may also arise from radiative decays from solar wind ions following charge exchange with neutral species in the cometary atmosphere – Stancil et al
- Recent comparisons of ionization cross sections between experiment and theory for O ions can be used by modelers to increase accuracy of model

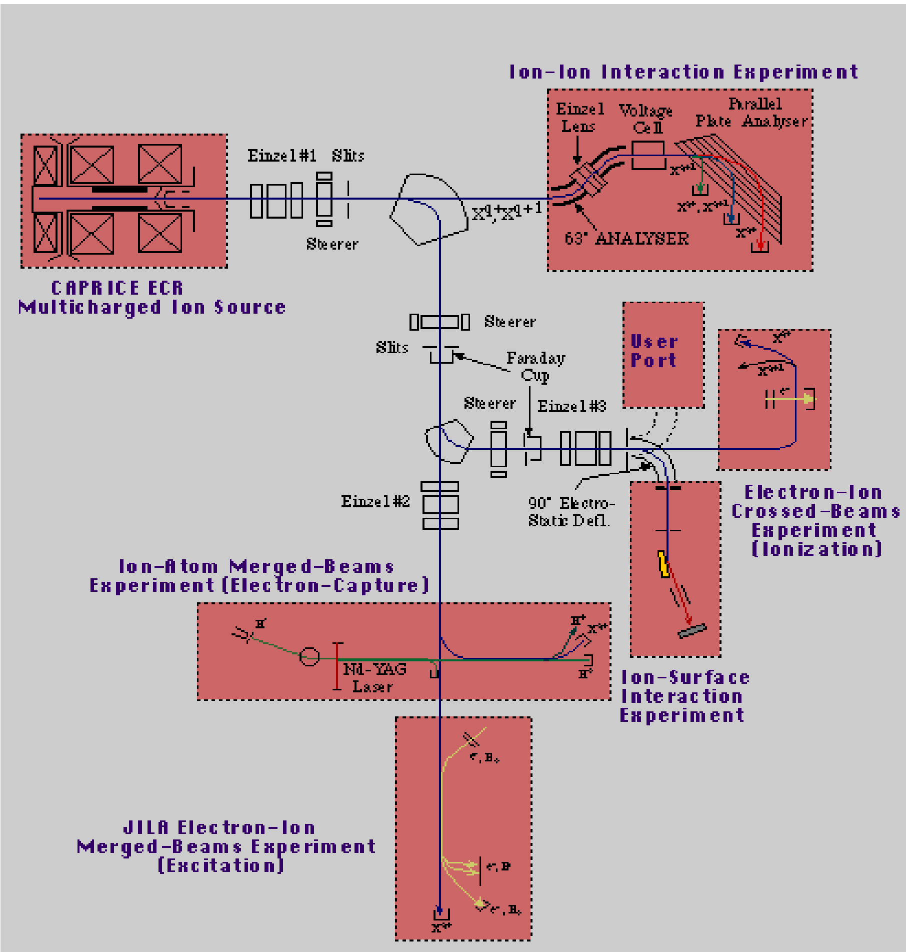


S. D. Loch et al, Phys. Rev. A 67, 042714 (2003).

Planned calculations

- Calculations of electron-impact ionization of ions in the Be-like, He-like and O-like isoelectronic sequences
- Many of these ions are directly observed by current X-ray observatories
- Ions in these sequences currently in astrophysical databases have significant uncertainties
- Theoretical calculations will support experiment; once theory and experiment agree, data will be used to produce more accurate ionization rate coefficients to be used in ionization balance calculations by astrophysical modelers
- Working closely with astrophysical modelers allows a guide to the systems which are important and selected for study

Electron-Impact Ionization Data for modeling cosmic plasmas

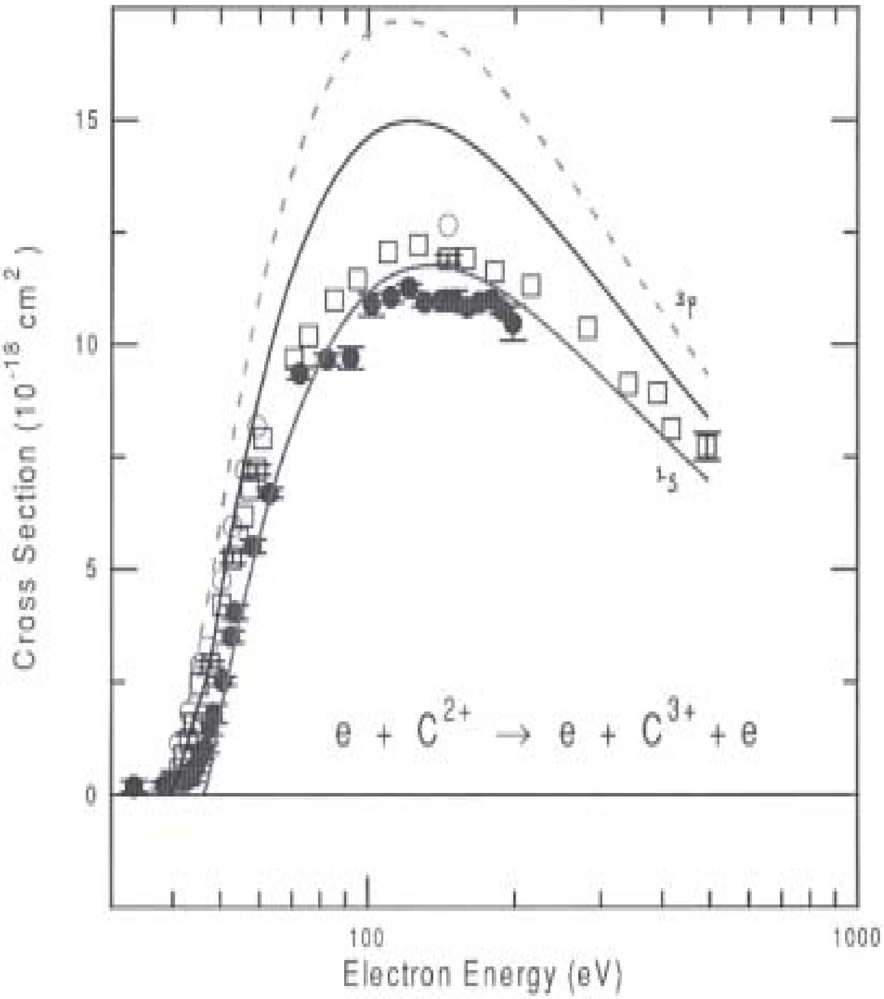


Outline of the MIRF (Multicharged Ion Research Facility) at ORNL, TN

- Detailed measurements are being planned at ORNL
- Unique facility in the U.S. as it measures both electron-impact excitation and ionization cross sections
- Allows measurements from metastable components of ion beams
- Major advance on previous measurements which could not give metastable component of ion beams - resulting in considerable uncertainties in the measurement

Future projects

$e^- + C^{2+} \rightarrow e^- + C^{3+} + e^-$



- Recent experiment of this process thought to be 40% ground (^{1}S) state and 60% metastable (^{3}P)
- Configuration-average distorted-wave calculations up to 30% higher than experiment
- Unclear if due to uncertainties in experimental determination of metastable fraction; new experimental measurements planned
- New calculations planned using TDCC method – though significant theory development required

Future directions – electron collisions with molecular ions

- Work in progress to calculate electron-impact excitation and ionization of light diatomic molecules
- Use time-dependent techniques; compare to *R*-matrix calculations
- Important in interactions of cosmic rays with atmospheric molecules
- Also diatomic molecules and molecular ions detected in interstellar clouds as well as in comets
- For many molecular species of astrophysical interest virtually no collisional data exists currently

Conclusions

- Discussed range of atomic & molecular processes which are important in accurately modeling fusion and astrophysical plasmas
- A series of theoretical techniques have been developed and implemented by our group to try to address some of these atomic physics issues
- Our aim is to work closely with astrophysical plasma modelers in order to provide quality atomic data for systems of interest
- Close collaboration and good communication between groups will enhance progress that will be made!